



Ultrafast Energy Transfer in Shocked Molecular Solids

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This research focuses on the interaction between shock waves and matter. In this work, we use classical molecular dynamics simulations to propagate shock waves through solid rare gas matrices containing an impurity. The first system studied is a diatomic embedded in an argon matrix. The diatomic is aligned both horizontally and diagonally, and the shock wave is propagated from the left, or up from the bottom. The resulting simulation data are analyzed and are found to exhibit much more complicated behavior than the previously studied one-dimensional model. The next system studied is an ozone molecule embedded in a solid neon matrix. When a shock wave is passed through this system, more complicated behavior results, including the formation of a void in the vicinity of the ozone molecule.

Introduction

- Use classical molecular dynamics simulations of model systems to study the effect of a soliton on an impurity molecule
- Vary the mass of the diatomic, and the velocities & direction of shock propagation. Qualitative interpretation and/or comparison with theory.
- Study the effect of soliton velocity on an ozone molecule in a neon lattice

Theory

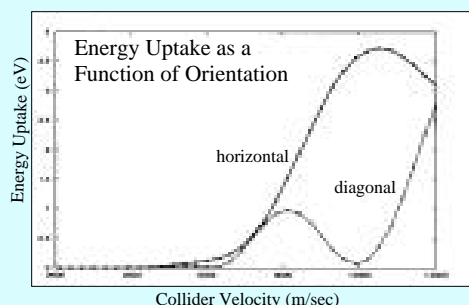
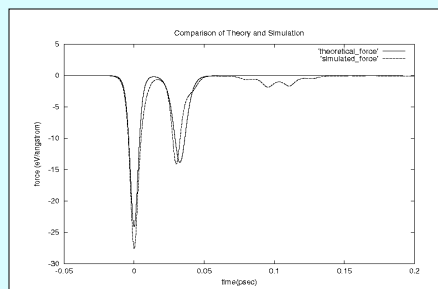
The theoretical force traces were generated by:

$$F(t) = F_1(t) + F_2(t - \tau)$$

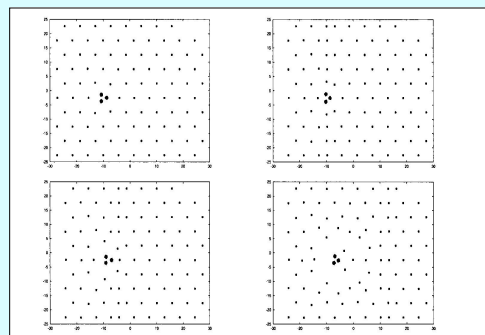
$$F_1(t) = -\frac{\alpha E_0}{L_0} \operatorname{sech}^2 \left(\frac{v_0 t}{2L_0} \right)$$

$$F_2(t - \tau) = -\frac{\alpha E_D}{L_f} \operatorname{sech}^2 \left(\frac{v_D(t - \tau)}{2L_f} \right)$$

Results



Void Formation Around Ozone Impurity



Future Directions

- Compare orientation effects using solitons with orientation effects using shock waves.
- Study the effect of shock waves on systems of energetic molecules.
- Include quantum mechanical effects in shock induced excitation of energetic molecules.